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# Prominent soft x-ray lines of Sr-like $Au^{41+}$ in low-energy EBIT spectrum

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**Abstract.** Relativistic multireference Møller-Plesset perturbation theory has been employed to calculate with high accuracy the energy levels and transition probabilities of Cu- to Sr-like gold ions. The many-body calculations were carried out to identify the unassigned blended lines in the 35–40 Å region of the low-energy EBIT spectrum of the gold ions [Träbert *et al* 2001 *Can. J. Phys.* **79** 153]. Most of the prominent lines in the 35–40 Å region were identified as the emission lines in Sr-like gold.

## 1. Introduction

In the last two decades, the electron-beam ion trap (EBIT) [1] has been successfully employed to produce well-resolved spectra of highly-ionized atomic ions. Using the Livermore EBIT-2, Träbert et al [2] obtained soft-x-ray spectra of Au with well-defined maximum charge states ranging from Br- to Co-like ions. The prominent lines in the spectra of Cu-, Zn-, Ga-, and Ge-like Au ions are well separated and they have been measured to very high accuracy – typically 0.01–0.005 Å. The line classifications for the strongest transitions in Cu-like to Rb-like Au were guided by theoretical calculations with the fully relativistic parametric potential code RELAC [3]. Typically the accuracy achievable with the large-scale RELAC calculations is of the order of 0.5–1.0 Å. Such an accuracy suffices to identify well-separated prominent lines. However, the complex EBIT spectra of Au ions produced at lower-energy electron beam contain numerous lines, many of which are blended. The uncertainties ($\approx$ 0.5–1.0 Å) in the extant theoretical predictions are too large to make unique line identifications of the line-rich spectra. We have recently developed and implemented a relativistic multireference Møller-Plesset (MR-MP) perturbation theory for high-accuracy calculations of spectroscopic quality for the term energies and decay probabilities of multi-valence-electron ions. The method was succesfully applied to calculate with high accuracy the spectra of Mg-, Al-, Si-, P-, Zn-, and Ga-like highly-ionized ions [4, 5, 6]. The theoretical predictions were within experimental uncertainties where available, with the estimated theoretical uncertainty of the order of 0.01 Å for the soft-x-ray lines.

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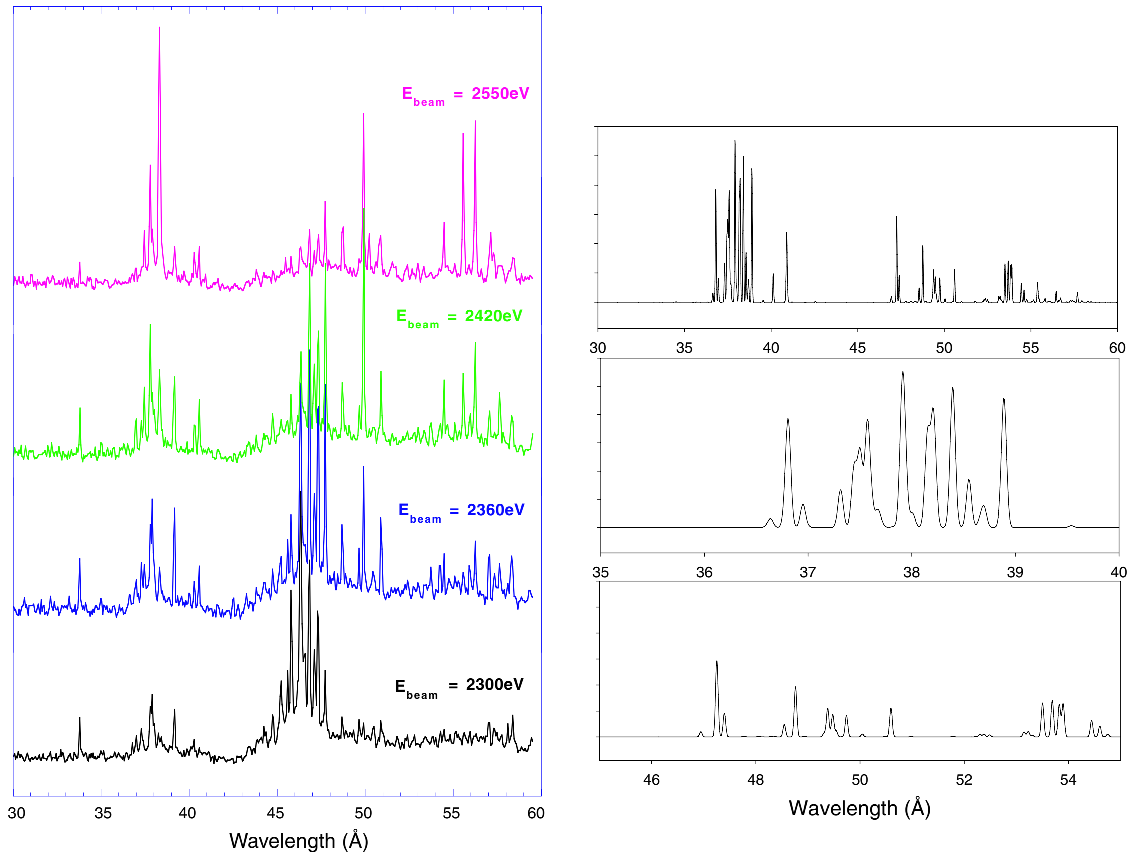


**Figure 1.** EBIT (left panel) and synthetic theoretical spectra (right panel) of gold ions in the wavelength range 30 to 60 Å. The two lower synthetic spectra are expanded sections of the upper one.

In the present study, our relativistic MR-MP perturbation theory calculations are employed to calculate with high wavelength accuracy the soft-x-ray spectra of Cu-like to Sr-like Au ions. The highly accurate theoretical predictions allow us to make immediate identifications of the individual lines in the line-rich EBIT spectra produced with a lower-energy electron beam.

## 2. Computational details

The state-averaged matrix multiconfiguration Dirac-Fock-Breit (MCDFB) self-consistent-field (SCF) calculations [7] were performed including 25 relativistic configuration state functions (CSFs) arising from the configurations, $4s^2 4p^6 4d^2$ and $4s^2 4p^5 4d 4f$. The state-averaged MCDFB SCF yield a single set of spinors for the ground and excited levels. Subsequently, each of the ground and excited states was subjected to state-specific second-order MR-MP refinement to account for the residual dynamic correlation. The reference space in the MR-MP refinement includes all the CSFs arising from the configurations $4s^{n1} 4p^{n2} 4d^{n3} 4f^{n4}$ with $n3 + n4 \leq 3$ and $n4 \leq 1$. Frequency-independent Breit correlation corrections were included in the second-order MR-MP. Frequency-dependent Breit correction, normal and specific mass shifts were evaluated at the first-order of perturbation theory. Lamb shift was estimated using the procedure proposed by Y.-K. Kim [8]. The even-tempered basis set of 26s24p22d20f18g18h Gaussian spinors for up to angular momentum $L = 5$ and 15 Gaussian spinors for $L = 6$–$11$ were employed.

**Table 1.** Energy levels (cm$^{-1}$) in strontiumlike Au$^{41+}$. In each level the occupation number of the seven relativistic shells $4s^{n1}4p_{1/2}^{n2}4p_{3/2}^{n3}4d_{3/2}^{n4}4d_{5/2}^{n5}4f_{5/2}^{n6}4f_{7/2}^{n7}$ of the dominant CSF is given in the columns denoted "Conf". The "Key" columns contain the $J$-value of the level and level number in parentheses. The odd-parity states are labeled by a star.

| Conf | Key | $E$ | Conf | Key | $E$ | Conf | Key | $E$ |
|---|---|---|---|---|---|---|---|---|
| 2242000 | 2(1) | 0 | 2231200 | 1(6)* | 1861503 | 2230300 | 3(17)* | 2218387 |
| 2242000 | 0(1) | 79342 | 2231200 | 3(8)* | 1870500 | 2230300 | 1(12)* | 2257805 |
| 2241100 | 3(1) | 204681 | 2231200 | 4(6)* | 1871604 | 2240110 | 3(18)* | 2264618 |
| 2241100 | 4(1) | 253344 | 2231200 | 4(7)* | 1881427 | 2240110 | 4(15)* | 2268037 |
| 2241100 | 2(2) | 254103 | 2241010 | 4(8)* | 1896611 | 2240110 | 2(18)* | 2275361 |
| 2241100 | 1(1) | 256919 | 2231200 | 3(9)* | 1899714 | 2240110 | 1(13)* | 2282086 |
| 2240200 | 4(2) | 455122 | 2231200 | 1(7)* | 1914565 | 2240110 | 0(6)* | 2293318 |
| 2240200 | 2(3) | 479178 | 2231200 | 4(9)* | 1915625 | 2230300 | 3(19)* | 2297888 |
| 2240200 | 0(2) | 547523 | 2231200 | 0(3)* | 1918328 | 2230300 | 4(16)* | 2307717 |
| 2233000 | 2(1)* | 1415793 | 2231200 | 2(9)* | 1931078 | 2230300 | 1(14)* | 2334544 |
| 2233000 | 1(1)* | 1432570 | 2231200 | 3(10)* | 1950097 | 2240101 | 2(19)* | 2337105 |
| 2233000 | 0(1)* | 1449330 | 2231200 | 2(10)* | 1969579 | 2240101 | 3(20)* | 2341707 |
| 2233000 | 3(1)* | 1461887 | 2231200 | 4(10)* | 1973026 | 2240101 | 1(15)* | 2416594 |
| 2232100 | 3(2)* | 1586356 | 2241010 | 2(11)* | 1976524 | 2143000 | 2(20)* | 2571374 |
| 2232100 | 2(2)* | 1603692 | 2231200 | 1(8)* | 1993166 | 2142100 | 3(21)* | 2697281 |
| 2232100 | 4(1)* | 1612828 | 2240110 | 3(11)* | 1996206 | 2142100 | 2(21)* | 2698800 |
| 2232100 | 2(3)* | 1625232 | 2240110 | 2(12)* | 1998282 | 2142100 | 1(16)* | 2702968 |
| 2232100 | 1(2)* | 1632158 | 2241001 | 4(11)* | 2012670 | 2142100 | 0(7)* | 2715509 |
| 2232100 | 3(3)* | 1643699 | 2240110 | 1(9)* | 2020271 | 2143000 | 1(17)* | 2716789 |
| 2232100 | 0(2)* | 1644150 | 2231200 | 3(12)* | 2020621 | 2142100 | 4(17)* | 2721642 |
| 2232100 | 4(2)* | 1645218 | 2231200 | 2(13)* | 2030829 | 2142100 | 2(22)* | 2840495 |
| 2232100 | 4(3)* | 1676686 | 2231200 | 0(4)* | 2031184 | 2141200 | 3(22)* | 2859169 |
| 2232100 | 2(4)* | 1681235 | 2231200 | 2(14)* | 2041432 | 2141200 | 4(18)* | 2871057 |
| 2232100 | 1(3)* | 1681833 | 2231200 | 1(10)* | 2059988 | 2141200 | 2(23)* | 2875402 |
| 2232100 | 3(4)* | 1684730 | 2241001 | 4(12)* | 2067437 | 2142100 | 3(23)* | 2885081 |
| 2241010 | 3(5)* | 1733525 | 2241001 | 3(13)* | 2067441 | 2141200 | 1(18)* | 2897648 |
| 2232100 | 4(4)* | 1734945 | 2230300 | 3(14)* | 2080723 | 2141200 | 0(8)* | 2897794 |
| 2232100 | 2(5)* | 1745994 | 2230300 | 0(5)* | 2082786 | 2141200 | 2(24)* | 2906140 |
| 2232100 | 2(6)* | 1771320 | 2231200 | 3(15)* | 2109897 | 2142100 | 4(20)* | 2907321 |
| 2232100 | 3(6)* | 1785742 | 2230300 | 2(15)* | 2116220 | 2142100 | 1(19)* | 2915616 |
| 2232100 | 1(4)* | 1805112 | 2241010 | 3(16)* | 2116380 | 2141200 | 3(24)* | 2921575 |
| 2231200 | 4(5)* | 1812558 | 2241010 | 1(11)* | 2130188 | 2142100 | 2(25)* | 2923354 |
| 2231200 | 2(7)* | 1817031 | 2241001 | 2(16)* | 2135655 | 2142100 | 3(25)* | 2933943 |
| 2232100 | 1(5)* | 1831439 | 2240101 | 4(13)* | 2138085 | 2141200 | 4(19)* | 2940595 |
| 2231200 | 3(7)* | 1854547 | 2230300 | 2(17)* | 2166047 | 2141200 | 2(26)* | 3008219 |
| 2231200 | 2(8)* | 1855055 | 2230300 | 4(14)* | 2174699 | 2140300 | 4(21)* | 3065255 |

## 3. Results and discussions

In Figure 1 the EBIT spectra of Au ions are compared with the simulated theoretical spectra of Sr-like Au ion. The synthetic spectra were produced by convoluting with gaussian function the line intensities proportional to "branched" transition probabilities, assuming a uniform level population. At the electron beam energies of 2300 eV there are two wavelength regions containing numerous lines within a 4–5 Å range. The first of these, in 37–40 Å region, was characterized in previous study [2] as containing multiple lines of Br-like Au. Our calculations predicted not a single Br-like gold line in that region, ruling out the posibility that those blends are lines of the Br-like ions. However, theoretical spectra in Figure 1 indicate that there are multiple lines of Sr-like gold blended in the 37–39 Å region (this region is shown separately in Figure 1). The many lines in the second wavelength region 45–48 Å are mostly unidentified. Relativistic MR-MP

**Table 2.** Identified lines in strontium-like $Au^{41+}$. The occupation of the seven relativistic shells $4s^{n1}4p_{1/2}^{n2}4p_{3/2}^{n3}4d_{3/2}^{n4}4d_{5/2}^{n5}4f_{5/2}^{n6}4f_{7/2}^{n7}$ in the dominant CSF of the upper and lower states is given in the columns denoted "Conf". The "Key" columns contain the J-value of the level and level number in parentheses. The odd-parity states are labeled by a star.

| $\lambda_{expt}$ Å | $\lambda_{theor}$ Å | Upper Conf | Upper Key | Lower Conf | Lower Key | $A$ $s^{-1}$ |
|---|---|---|---|---|---|---|
| 37.42 | 37.443 | 2141200 | 1(18)* | 2241100 | 2(2) | 1.46(+12) |
| 37.75 | 37.702 | 2141200 | 1(21)* | 2240200 | 2(3) | 5.32(+11) |
| 38.00 | 37.939 | 2142100 | 3(23)* | 2241100 | 3(1) | 1.21(+12) |
| | 37.910 | 2141200 | 1(22)* | 2240200 | 0(2) | 2.60(+12) |
| | 37.915 | 2143000 | 1(17)* | 224200 | 0(1) | 1.61(+12) |
| | 38.009 | 2142100 | 3(23)* | 2241100 | 2(2) | 6.13(+11) |
| 38.26 | 38.210 | 2141200 | 2(27)* | 2240200 | 2(3) | 2.47(+12) |
| 38.35 | 38.396 | 2141200 | 1(20)* | 2241100 | 2(2) | 3.10(+12) |
| 38.60 | 38.552 | 2142100 | 2(22)* | 2241100 | 2(2) | 1.08(+12) |
| | 38.699 | 2141200 | 1(21)* | 2240200 | 0(2) | 5.91(+11) |
| 47.27 | 47.251 | 2241010 | 1(11)* | 2242000 | 2(1) | 2.00(+12) |
| 48.64 | 48.760 | 2141200 | 1(21)* | 2242000 | 0(1) | 1.61(+12) |

calculations were performed to examine if the Sr-like gold ion has any strong radiative emission in that region. The synthetic spectrum has just two prominent lines of Sr-like gold at 47.251 Å and 48.760 Å. The remaining lines instead relate to other charge states such as Y-like Au ions. In the ions of partially occupied $4d$ shell, numerous low-lying excited states have term energies nearly degenerate with the ground state. The branching of the decays of the higher-lying excited states to the ground state and to the low-lying excited levels produce multiple prominent lines in the same wavelength region. Table 1 lists term energies of the lowest 48 levels. It is clear that decays of the same upper state to the ground state and lowest five even-parity states produce E1 lines in the same wavelength region and highly accurate theoretical predictions must be brought to bear (accurate to 0.05Å) to identify the lines in such a line-rich spectrum. Table 2 displays the Sr-like gold lines identified by the present theoretical work.

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